

Statistical Software for Gradient Experiments

Walter Liggett

Statistical Engineering Division, NIST

Michael Wang

Polymers Division, NIST

Sharing Data Analysis Approaches

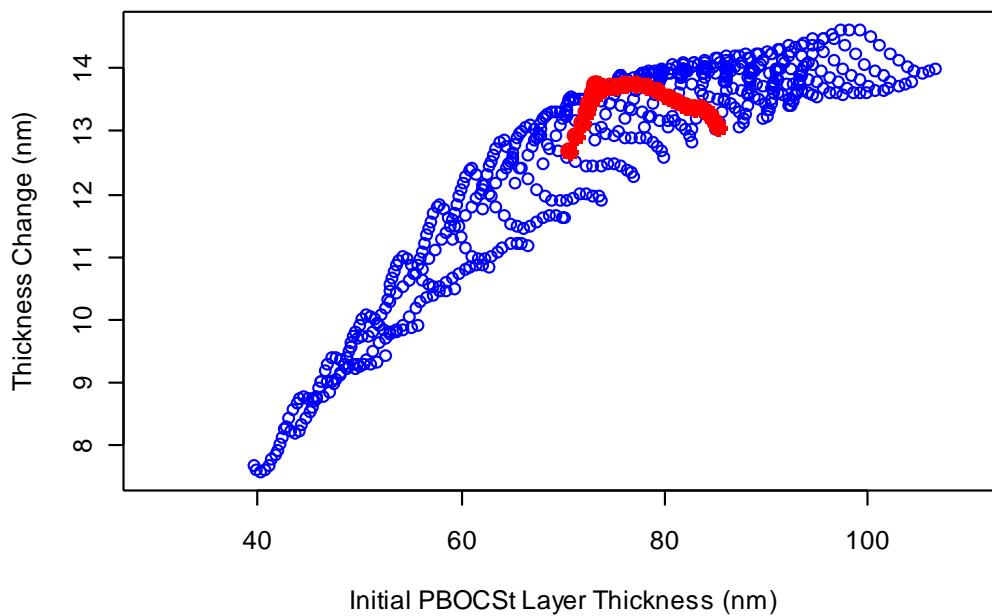
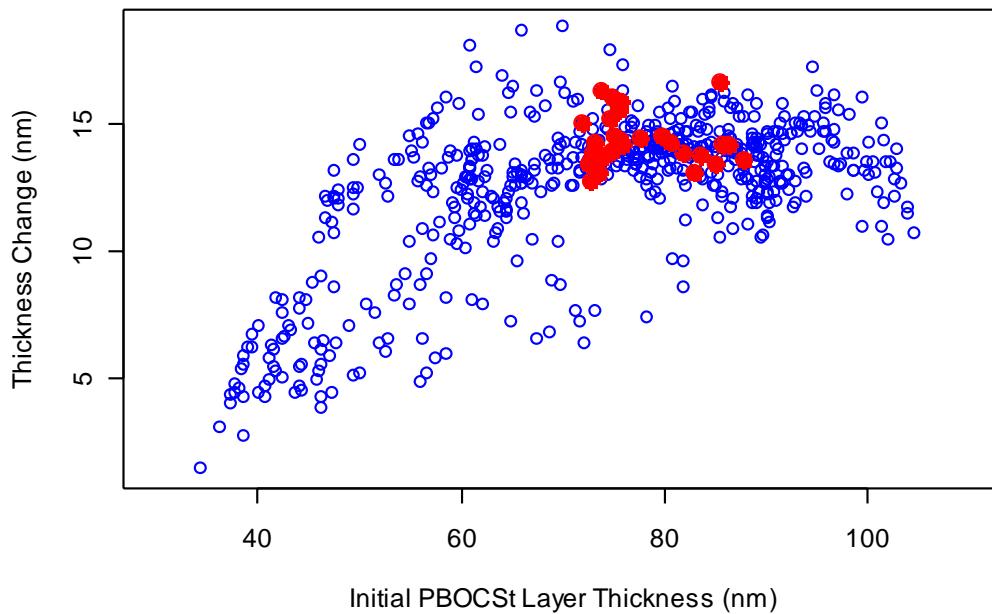
- An illustration of the need for statistics capability: Separation of the smooth from the rough in a gradient experiment
- R: a capable statistical package that is worth the effort to learn
- Sharing an approach by describing the arguments of the R functions used

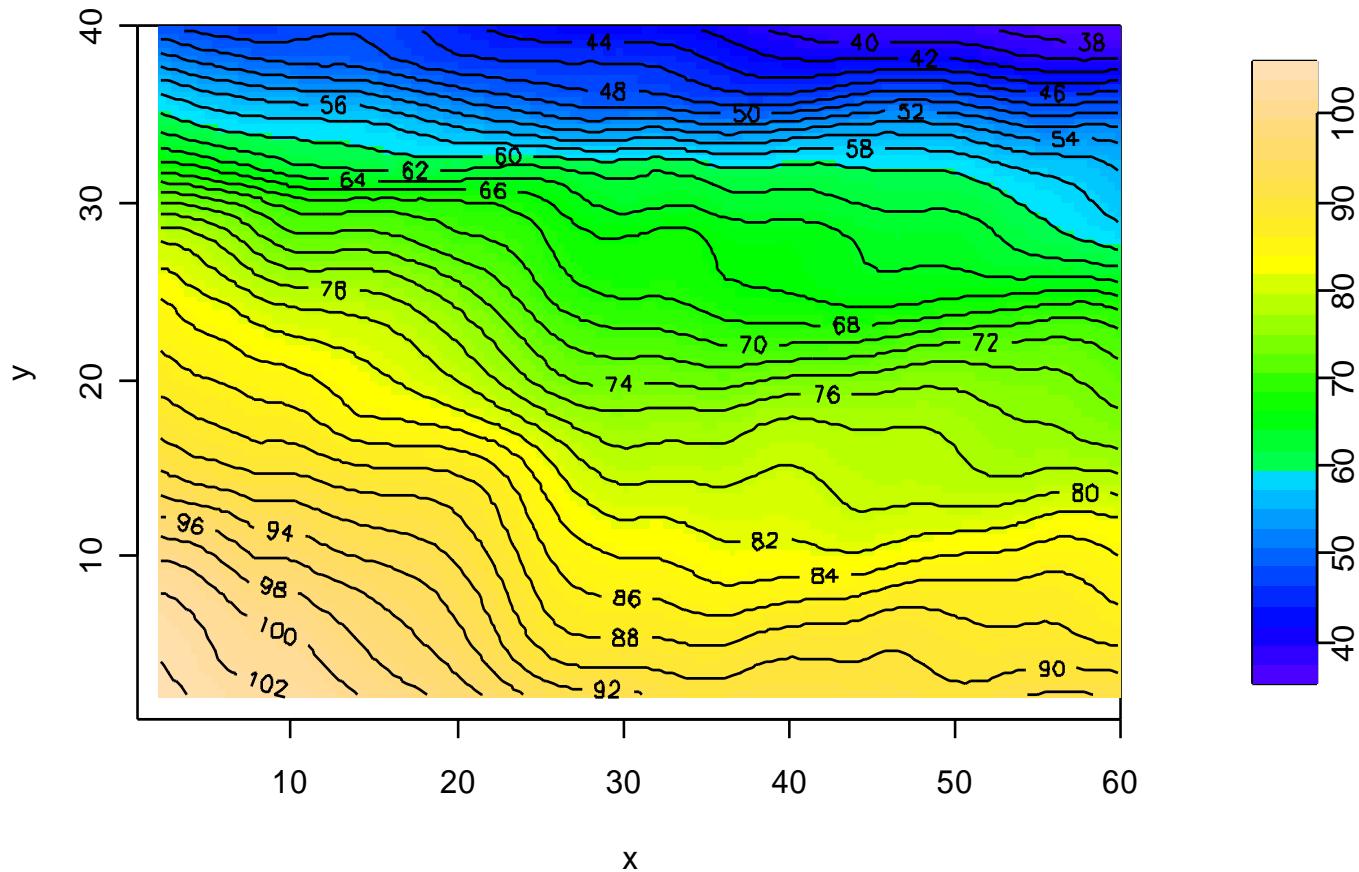
Mathematical Model

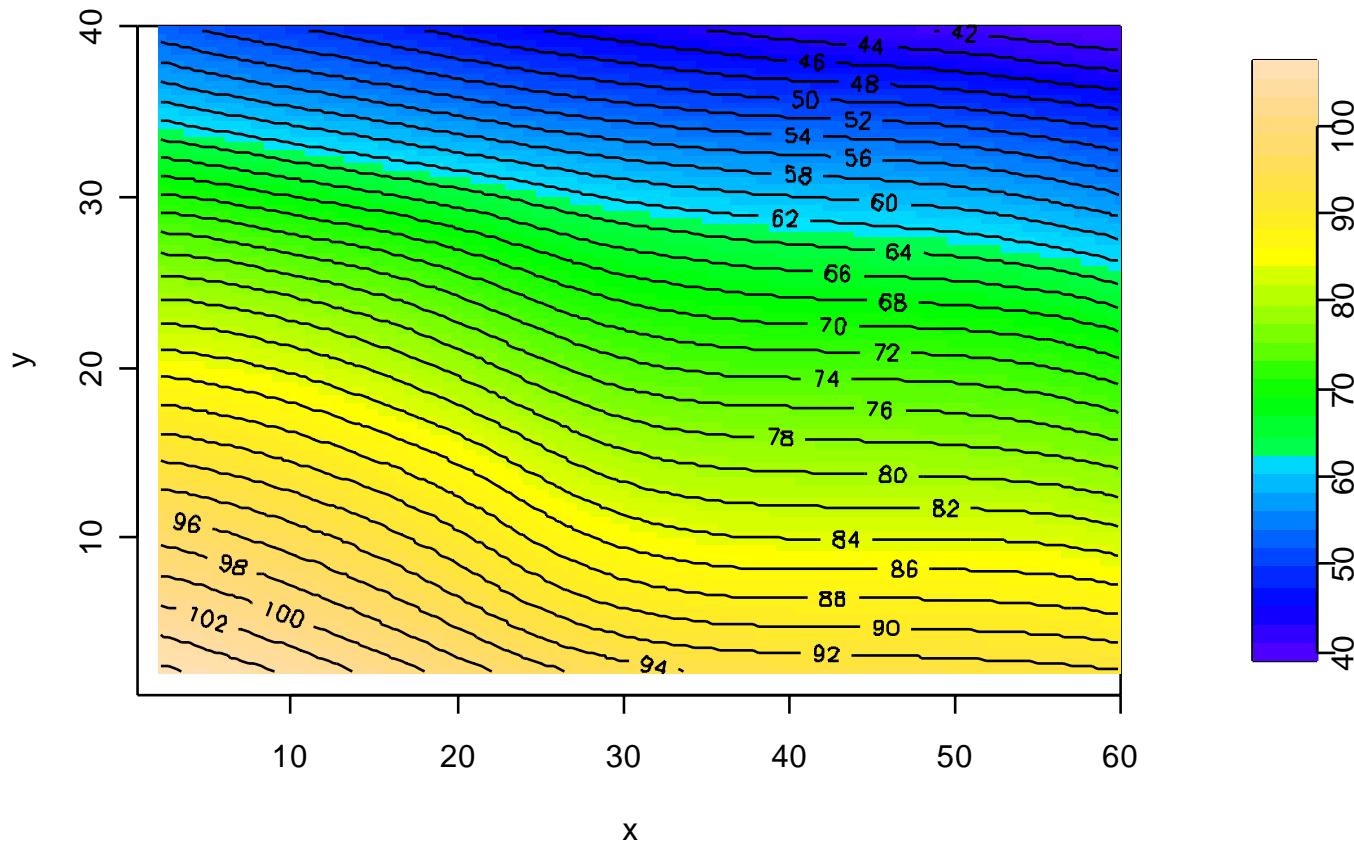
- Grid positions $x_i, y_i, i = 1, \dots, n$
- Before

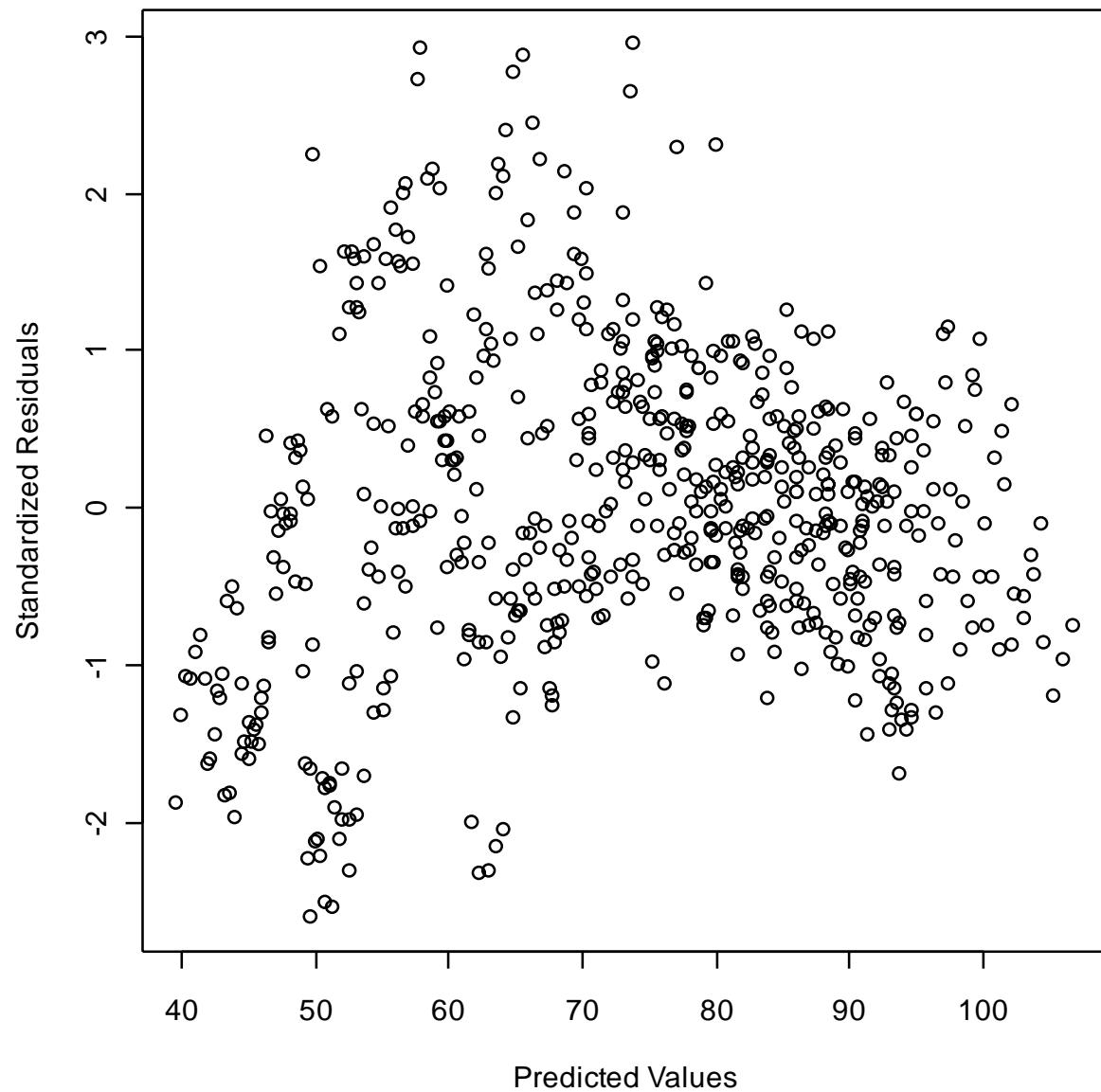
$$z_{1i} = d(x_i, y_i) + e_{1i}$$

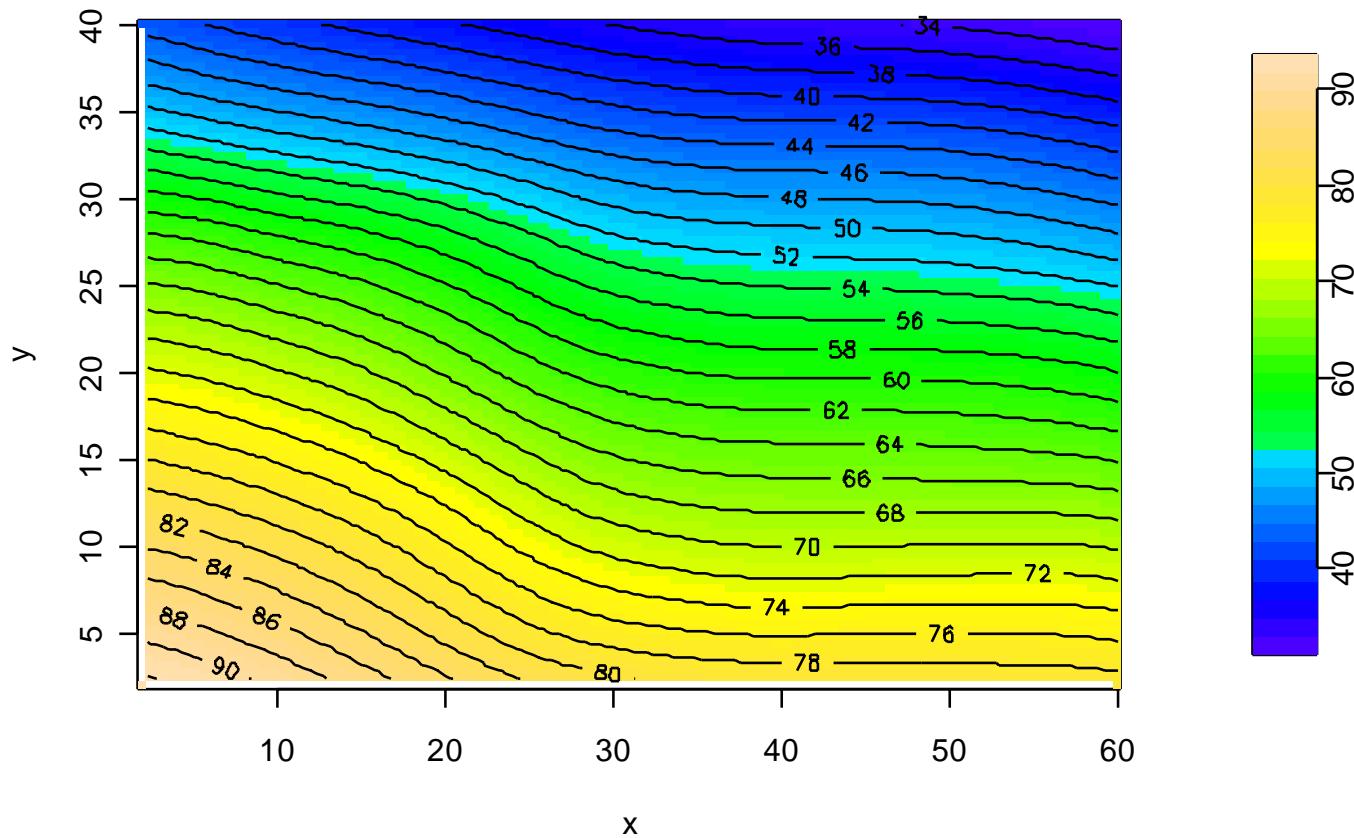
- After
- Plot of $z_{1i} - z_{2i}$ versus z_{1i}
- Implications of smoothness

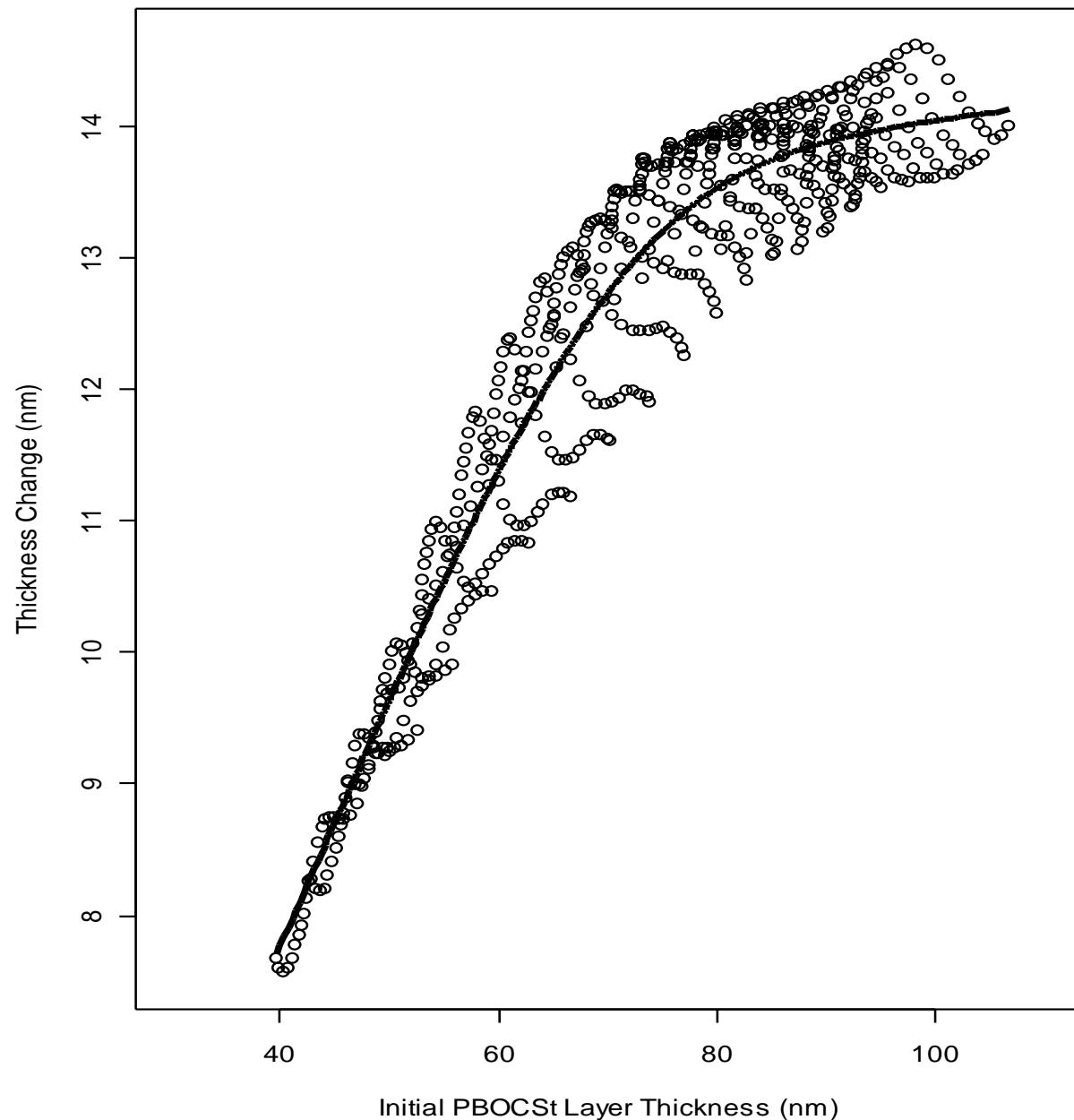


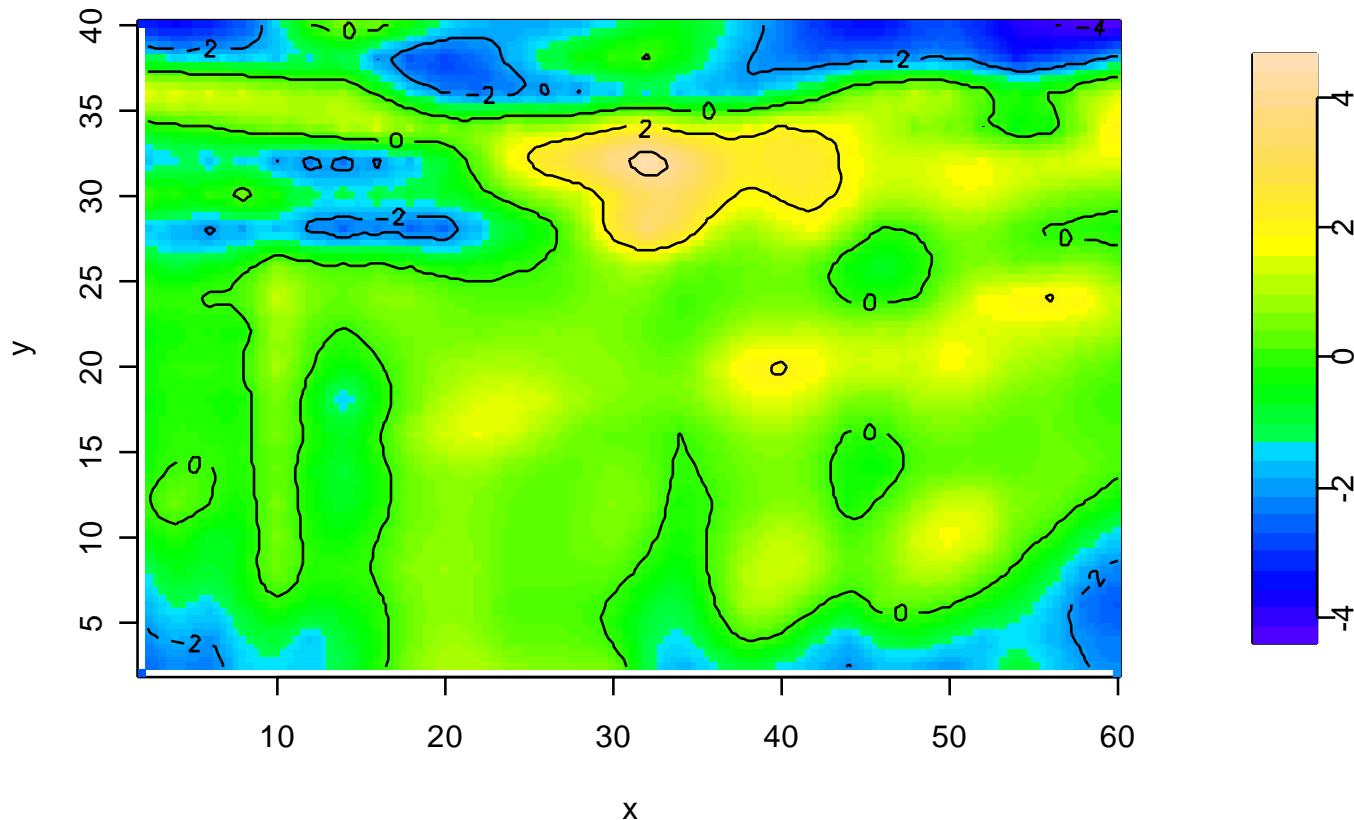












R

- Venables and Ripley (2002), Springer
- <http://lib.stat.cmu.edu/R/CRAN>
- R package “fields”
- Same commands as S-PLUS

Manipulating Data

```
Tgb <- as.vector(Thickgradb)
Tga <- as.vector(Thickgrada)

xmm <-
cbind(rep(seq(2,60,2),20),rep(seq(2,40,2),rep(30,
20)))
dimnames(xmm)[[2]] <- c("x","y")
```

Contour Plots

```
fitbs200 <-
Krig(xmm,Tgb,exp.cov,theta=c(16,16),df=200).

gl <- list(x=seq(2,60,.4),y=seq(2,40,.4))
surface.Krig(fitbs200,grid.list=gl,type="C",level
s=seq(30,110,2))
```

Fitting Line

```
diff <- fitbs20$fitted.values-
fitas20$fitted.values
plot(fitbs20$fitted.values,diff).

sreg4 <- sreg(fitbs20$fitted.values,diff,df=4)
```

Smoothing Residuals

```
res4 <- Tgb - Tga - sreg4$fitted.values  
fitres <-  
Krig(xmm,res4,exp.cov,theta=c(16,16),df=200)
```

Selection of Statistical Software

- Data analysis: creative matching of generic approaches with an individual data set
- Tradeoff between software capability and ease of learning
- Learning to use R
 - Perform operations one already knows
 - Apply unfamiliar statistical methods